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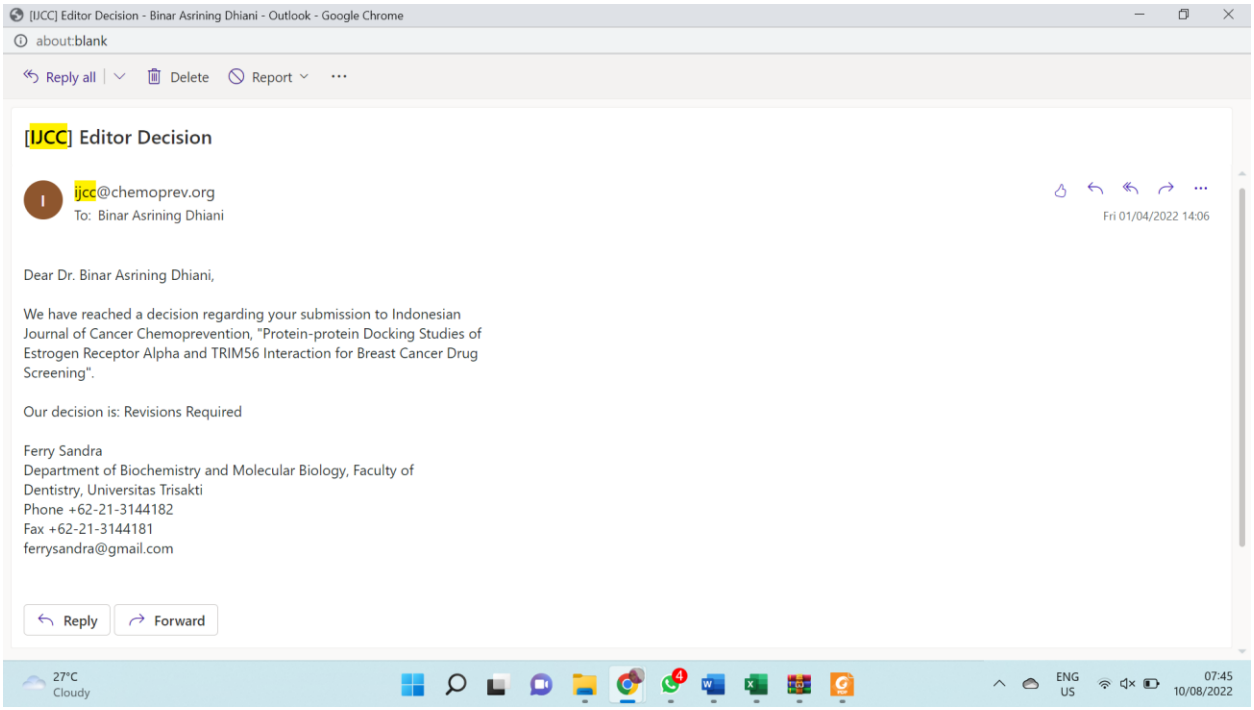

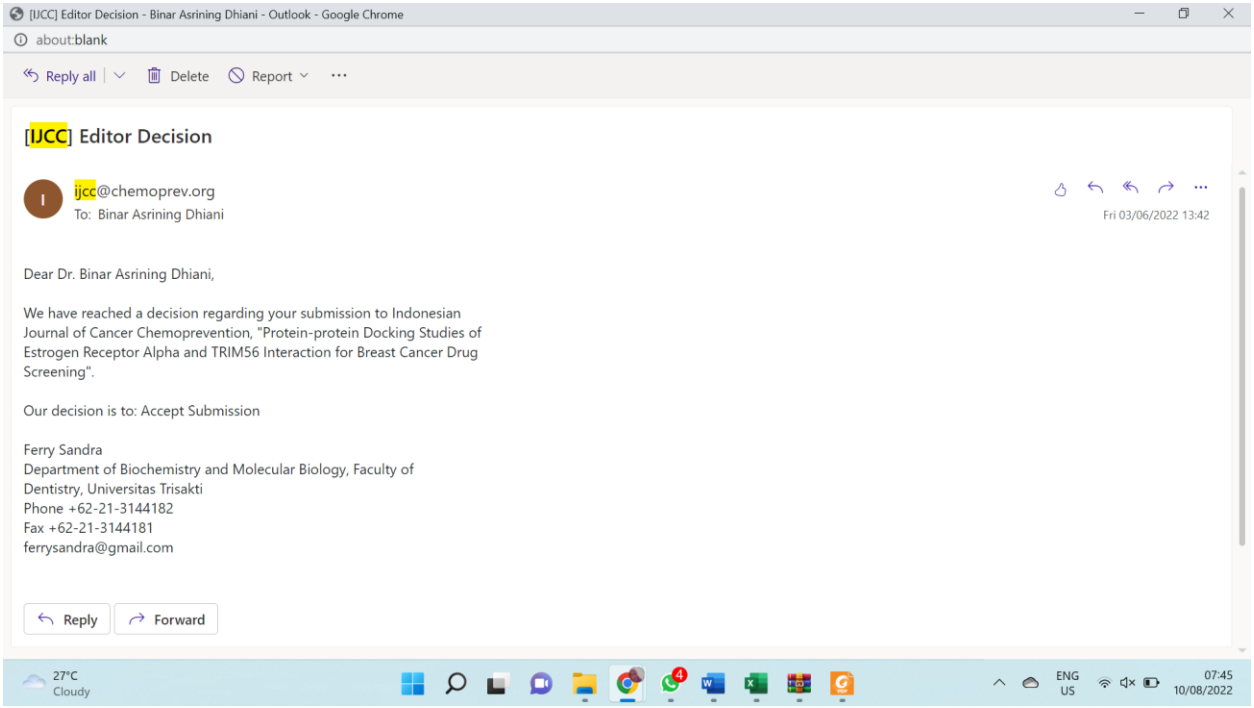

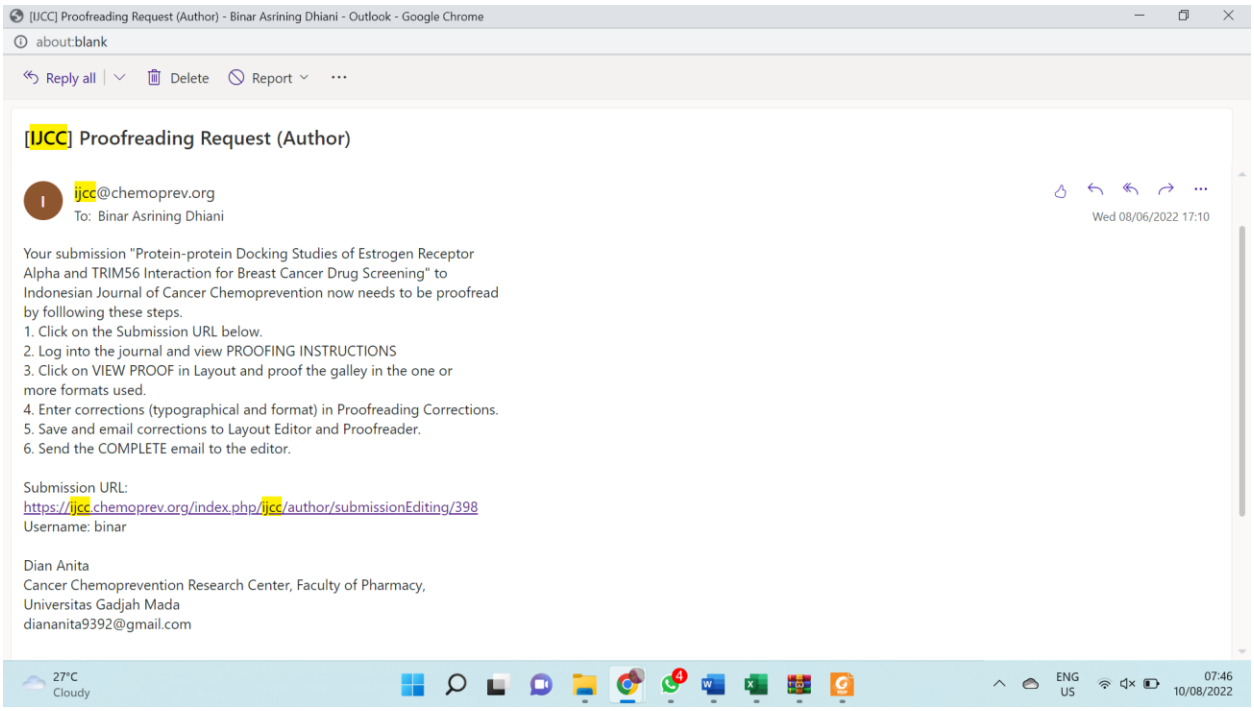
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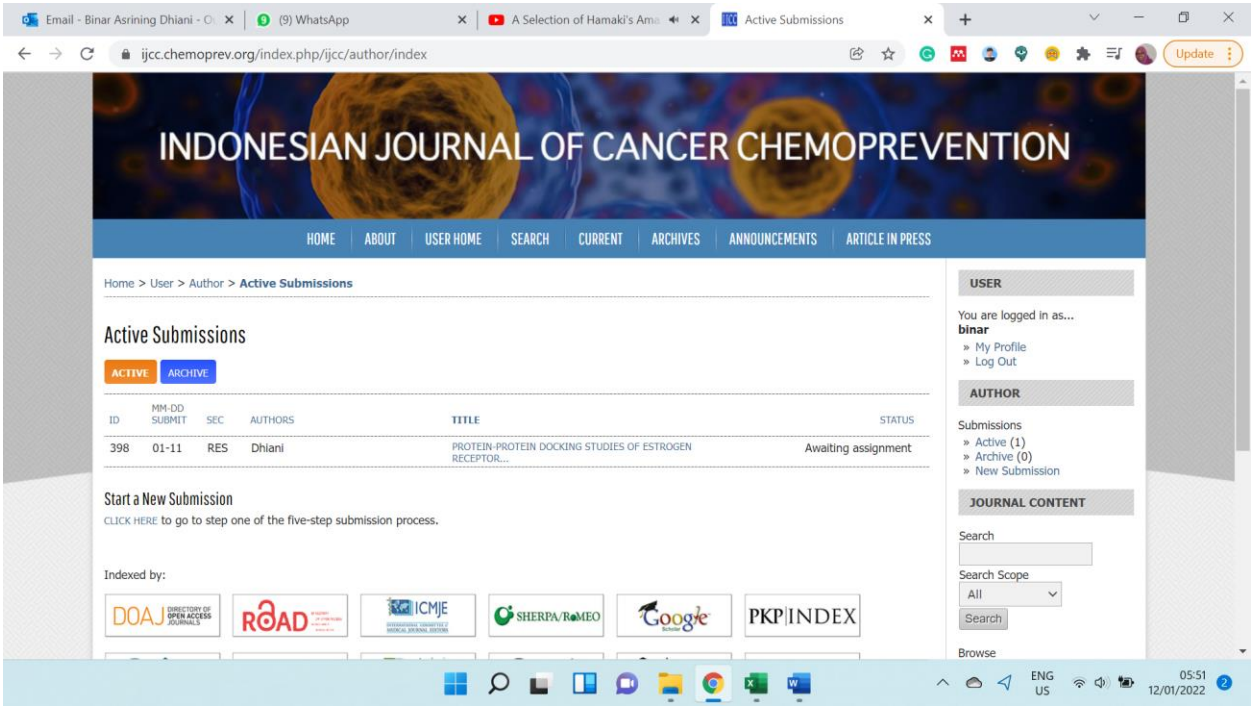
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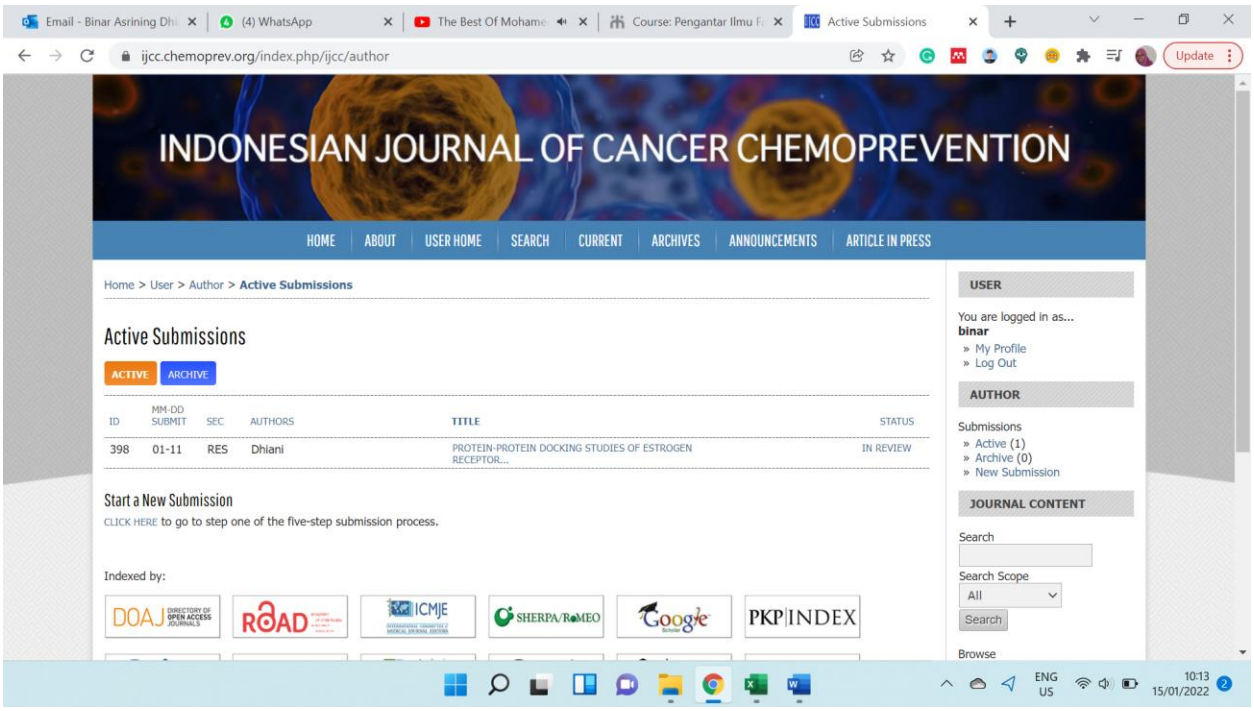
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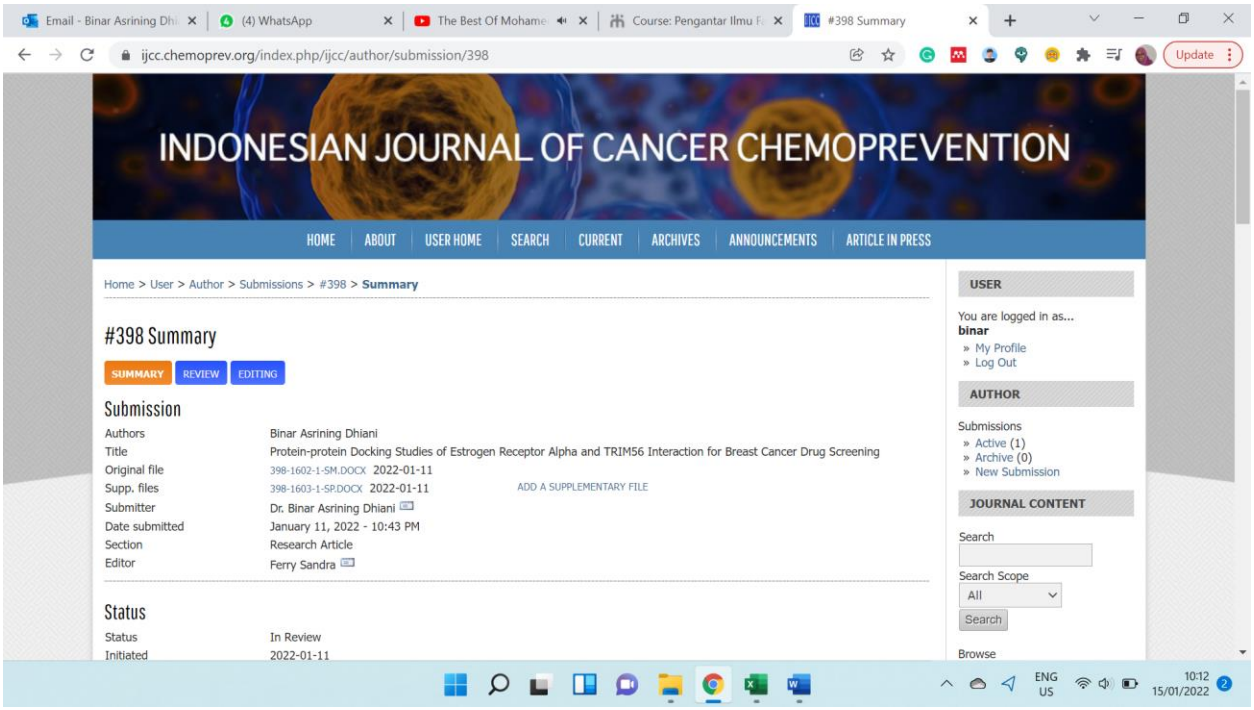
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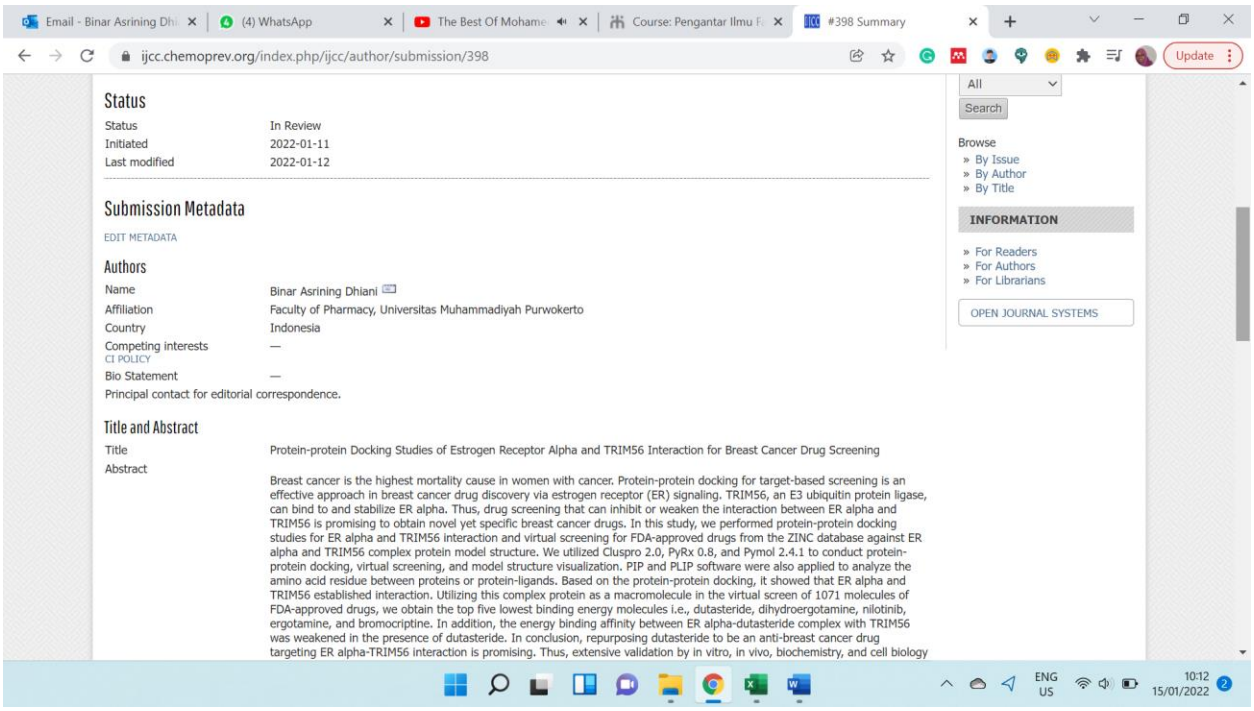

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Submission Metadata

EDIT METADATA

Authors

Name	Binar Asrining Dhiani
Affiliation	Faculty of Pharmacy, Universitas Muhammadiyah Purwokerto
Country	Indonesia
Competing interests CI POLICY	—
Bio Statement	—

Principal contact for editorial correspondence.

Title and Abstract

Title: Protein-protein Docking Studies of Estrogen Receptor Alpha and TRIM56 Interaction for Breast Cancer Drug Screening

Abstract:

Breast cancer is the highest mortality cause in women with cancer. Protein-protein docking for target-based screening is an effective approach in breast cancer drug discovery via estrogen receptor (ER) signaling. TRIM56, an E3 ubiquitin protein ligase, can bind to and stabilize ER alpha. Thus, drug screening that can inhibit or weaken the interaction between ER alpha and TRIM56 is promising to obtain novel yet specific breast cancer drugs. In this study, we performed protein-protein docking studies for ER alpha and TRIM56 interaction and virtual screening for FDA-approved drugs from the ZINC database against ER alpha and TRIM56 complex protein model structure. We utilized Cluspro 2.0, PyRx 0.8, and Pymol 2.4.1 to conduct protein-protein docking, virtual screening, and model structure visualization. PIP and PLIP software were also applied to analyze the amino acid residue between proteins or protein-ligands. Based on the protein-protein docking, it showed that ER alpha and TRIM56 established interaction. Utilizing this complex protein as a macromolecule in the virtual screen of 1071 molecules of FDA-approved drugs, we obtain the top five lowest binding energy molecules i.e., dutasteride, dihydroergotamine, nilotinib, ergotamine, and bromocriptine. In addition, the energy binding affinity between ER alpha-dutasteride complex with TRIM56 was weakened in the presence of dutasteride. In conclusion, repurposing dutasteride to be an anti-breast cancer drug targeting ER alpha-TRIM56 interaction is promising. Thus, extensive validation by in vitro, in vivo, biochemistry, and cell biology assays, is crucial to strengthen this evidence.

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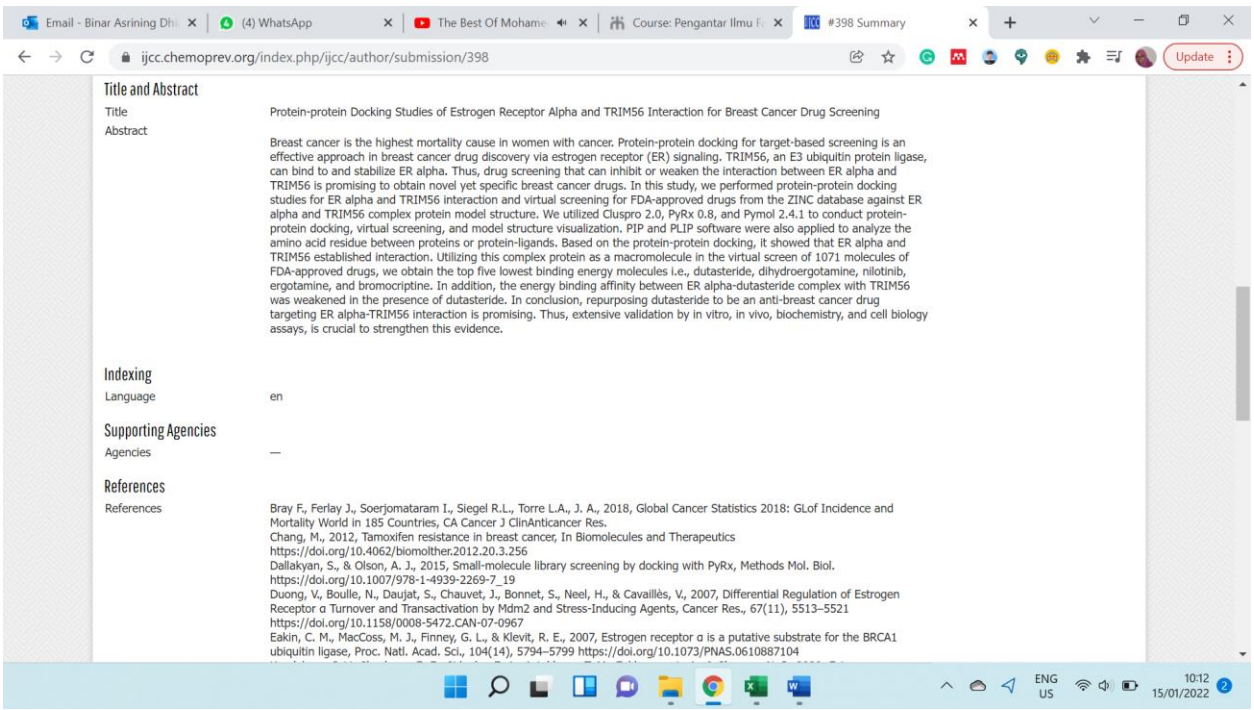

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Indexing

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Supporting Agencies

Agencies: —

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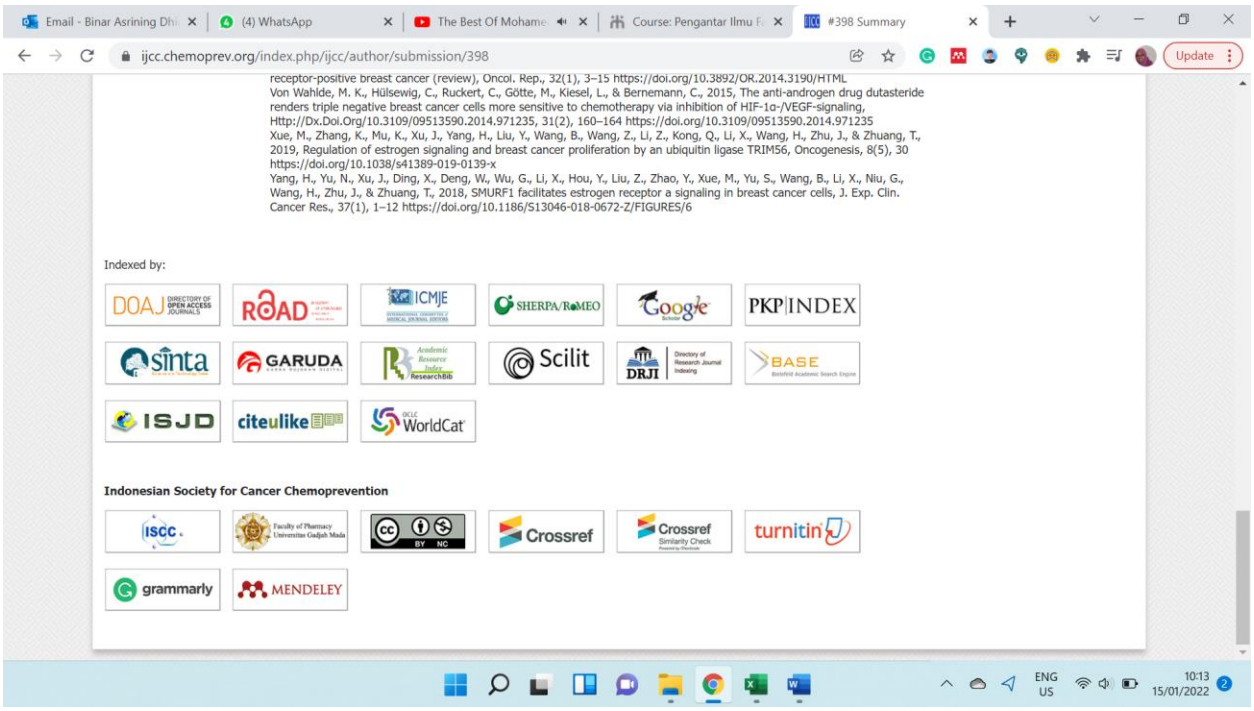
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Author response on reviewer comments

Title: Protein-protein Docking Studies of Estrogen Receptor Alpha and TRIM56 Interaction for Breast Cancer Drug Screening.

Thank you for all concerns raised by the reviewers. All comments are beneficial to improve the quality of the article. The author's responses to each comment are as follow:

REVIEWER #1

1. **Comment:**

   Abstract: repurposing should be avoided.

   Response:

   The author does not really understand what the reviewer meant regarding the comment suggesting that "repurposing should be avoided". Is it; (1) the repurposing dutasteride to be anti-breast cancer that should be avoided scientifically? Or, (2) the wording 'repurposing dutasteride' in the abstract that should be avoided to be expressed as a conclusion?

   If the reviewer means is, the repurposing dutasteride to be anti-breast cancer that should be avoided scientifically, then we would like to provide the evidence showing the attempt of drug discovery scientists in the world to repurpose the existing and market-available drugs (either oncology drugs or non-oncology drugs) for anti-breast cancer.

   Malik et al (2022) listed in their review in Table 4. about drugs that are repurposed and approved for breast cancer which includes several chemicals with original indications for prostate cancer, ovarian cancer, and colon cancer (https://www.sciencedirect.com/science/article/pii/S0753332221011598). In addition, Pantziarka et al (2018) mentioned terminology 'soft repurposing' for characterization of re-use of existing oncological drugs and 'hard repurposing' for the use of non-cancer drugs as anti-cancer medications. So, it is supported that 'repurposing' is appropriate scientific terminology for dutasteride to be used as anti-breast cancer (please see https://www.frontiersin.org/articles/10.3389/fphar.2018.00637/full).

   However, if the reviewer means is, that the wording 'repurposing dutasteride' in the abstract that should be avoided to be expressed as a conclusion of this study, then we are agreed and made a correction in the abstract section (page 1 line 19-21).

2. **Comment:**

Introduction section lacks protein-protein docking significance and how important this method for drug screening.

Response:

We added the requested information on page 2 lines 3-9.

3. **Comments**

Methods:

a. The second paragraph of this section contains “dan”.

Response:

We corrected “dan” to be “and”.

b. No proteins and FDA-approved drugs preparation were mentioned in the manuscript.

Response:

We added the preparation of 5JW7 (TRIM56) and 1A52 (ER alpha) proteins and FDA-approved drugs information as requested in the Methods section page 3.

c. No information of the native ligands for 5JW7 (TRIM56) and 1A52 (ER alpha).

Response:

We added the information of 5JW7 (TRIM56) and 1A52 (ER alpha) native ligand as requested in the Methods section page 3.

d. It is not clearly stated how to validate the protein-protein docking of ERα and TRIM56.

Response:

We added the information how to validate the best cluster model structure of ERα and TRIM56 in the method section.

e. Please provide the reference(s) for the parameter of optimization of 1615 FDA-approved drugs so that only 1071 molecules were selected.

Response:

We added the detail and a reference for energy optimization parameters for these 1615 FDA-approved drugs as requested in the Methods section page 4 line 10-14. For the note, 1071 molecules were generated automatically from the energy minimization process performed by Open Babel assembled in PyRx 0.8 tools and the author have not performed and applied any other selection parameters.

4. Results:

a. Natural ligand or native ligand?.

Response:

Yes, it should be native ligand. We have corrected it.

b. Please provide the complete name of the residues for all interactions between ER alpha and TRIM56.

Response:

We have provided the full name of the residues as requested.

c. 1615 FDA-approved drugs or 1651 FDA-approved drugs?.

Response:

The correct number is 1615 and we have corrected it in the manuscript.

d. Please check the second sentence in the second paragraph of the second part of this section.

Response:

We have checked and made a correction.

e. Please check the caption of Figure 3.

Response:

We have checked and made a correction.

f. Results section should be clear and concise, displays and is constructed based on the obtained data.

Response:

We made corrections needed to improve clarity and conciseness

5. Discussion:

a. Discussion is not a section for literature review but interprets the results including generalizability and limitation of the research.

b. Discussion does not repeat the description of the results.

c. Discussion concludes with a brief paragraph highlighting the main points of the study, including a statement regarding the translational value of the work.

d. Discussion is also clear to the readers especially non-specialist.

Response:

We made corrections to fulfill the requested content in the discussion section

6. Conclusion states the significance of the study and its potential impact in the field supported by the results. Conclusion should also lead the reader to the most important information from the manuscript.

Response:

We fulfilled the requested information.

7. References; please look at the author guideline.

   Response:

   We have made a correction to follow the author's guideline.

8. Please revised the whole manuscript to meet the standard of scientific article.

   Response:

   We have made the correction, revisions, and additional information in the manuscript to meet the standard.

REVIEWER #2

Responses:

1. We deleted '…, it showed that…' in the abstract.
2. We made corrections on the in-text citing style.
3. We made the correction in the consistency on writing style for ER alpha and ER beta in the manuscript.
4. We have added the URL of the Cluspro 2.0 web server.
5. We have added the URL of the PyRx 0.8.
6. We can not provide the URL of AutoDock Vina as we used the AutoDock Vina that is assembled in PyRx 0.8 tools.
7. We have added the URL of the FTMap web server.
8. We have added the URL of the PyMol software source
9. We made corrections to the first section of the first paragraph in the result.
10. Comment: Is this weighted score only represent by number or is there accompanying unit?

    Response: Yes, the weighted score that is coming from Piper in the ClusPro 2.0 is only a number without any unit.

11. Comment: (The protein interface analysis using PIC) Not mentioned in the Methods. Should be mentioned in Methods section as well.

    Response: We have added the information in the Methods section as requested.

12. Comment: In Table 1 the amino acid is written in the all-capital format, while here in not (capital only the first letter). I think either way is acceptable as long as is CONSISTENT throughout the article.

    Response: We made a correction on the amino acid name writing by using the full name of the amino acids with the capital letter in the first letter.

13. Comment: The author(s) has described dutasteride very well. If the author(s) can add a brief description for other 4 drug candidates it will be even better. It is already stated in the Table S2, but a brief description maybe needed in the main text.

    Response: We added the requested brief descriptions in the discussion section.